

**COMPUTATIONAL FLUID DYNAMICS OF FLOODING, LOADING  
AND FULLY DISPERSED REGIME IN GAS-LIQUID STIRRED  
TANK**

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## ABSTRACT

The main aim of this work is to perform computational fluid dynamics on gas-liquid stirred tank operating under flooding, loading and fully dispersed regime. This computational method was conducting with the combination of computational fluid dynamics (CFD) and drag model changes by using standard FLUENT model. This current work was attempted to predict the gas hold-up and gassed power number similarly like the result obtained by Ford et al. (2008). The overall research methodology consists of two main steps. First step is about drawing the gas-liquid stirred tank geometric and set the set-up and for the second step is about analysis the flow in gas-liquid stirred tank. After the boundary and the tank geometry have been set up, the selected mathematical model were employed; in the multiphase model, Eulerian-Eulerian model has been used while in turbulence model, two-phase standard k- $\epsilon$  has been employed. Besides that, the drag model of bubble by Schiller & Naumann (1935) was carried out. Diameter of bubbles is taken into account by employed the equation of *Sauter* mean diameter proposed by Calderbank (1958). The gassed power number and gas hold-up inside gas-liquid stirred tank were found to be in fair agreement to the experimental data adopted from Ford et al. (2008). The advantages of this computational method are the operating cost is lower compared to experimental method and besides, it can reduce the time taken to evaluate the performance of gas-liquid STR by neglecting the prototype's design. Through this study, CFD model may be useful to eliminate the impeller flooding in gas-liquid STR.

**Keywords:** CFD; gas-liquid; Hold-up; gassed power number; flooding

## ABSTRAK

Tujuan utama kerja ini adalah untuk melaksanakan pengiraan dinamik bendalir (*Computational Fluid Dynamics, CFD*) pada gas-cecair dikacau di dalam tangki yang beroperasi di bawah kawasan banjir, pemuatan dan sepenuhnya bersurai. Kaedah pengiraan ini telah menjalankan dengan kombinasi dinamik bendalir pengiraan (*CFD*) dan seret perubahan model dengan menggunakan model FLUENT standard. Semasa kerja ini, ia cuba meramalkan gas memegang dan kuasa nombor gas yang sama seperti keputusan yang diperolehi oleh Ford et al. (2008). Metodologi penyelidikan keseluruhan terdiri daripada dua langkah utama. Langkah pertama ialah melukis geometri cecair gas dikacau tangki dan menetapkan set-up dan untuk langkah kedua ialah menganalisis aliran cecair gas tangki dikacau. Selepas sempadan dan geometri tangki telah direka, model matematik yang dipilih akan digunapakai dalam model yang berbilang-fasa, model *Eulerian-Eulerian* telah digunakan semasa dalam model gelora, dua fasa standard k- $\epsilon$  juga telah digunakan. Selain itu, model seretan gelembung oleh Schiller & Naumann (1935) telah dijalankan. Diameter buih diambil kira dengan menggunakan persamaan diameter min Sauter yang dicadangkan oleh Calderbank (1958). Bilangan pengudaraan kuasa dan gas tahan dalam cecair gas dikacau tangki didapati dalam perjanjian yang adil kepada data uji kaji yang diguna pakai dari Ford et al. (2008). Kelebihan kaedah ini pengiraan kos operasi lebih rendah berbanding dengan kaedah eksperimen dan selain itu, ia boleh mengurangkan masa yang diambil untuk menilai prestasi STR gas-cecair dengan mengabaikan reka bentuk prototaip. Melalui kajian ini, model CFD mungkin berguna untuk menghapuskan banjir pendesak dalam STR cecair gas.

*Kata kunci:* CFD; gas-cecair; gas memegang; bilangan kuasa pengudaraan; banjir

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## LIST OFSYMBOLS

$a_i$	Interfacial area
$\alpha$	Constant (Eq. 2.12)
$\alpha_g$	Gas hold up
$\alpha_l$	Liquid volume fraction
$\beta$	Constant (Eq. 2.12)
$C$	Clearance
$C$	Dimensionless shape factor (Eq. 2.2)
$C_D$	Drag coefficient
$C_L$	Lift coefficient (Eq. 3.3)
$C_{\varepsilon 3}$	Constant equation (Eq.3.14)
$D$	Tank diameter
$d_{32}$	<i>Sauter</i> mean diameter
$d_{bi}$	Local bubble diameter
$d_{bs}$	<i>Sauter</i> mean diameter
$\varepsilon$	Energy dissipation
$\varepsilon_g$	Local gas hold up
$F_{lg}$	Gas flow number
$Fr$	Froude number
$F_{\beta\alpha}$	Interaction forces between continuous and dispersed phase

$\vec{F}_{lg}$	Interaction force per unit volume
$\vec{F}_{lift,l}$	Lift force
$\vec{F}_{vm,l}$	Virtual mass force
$g$	Gravitational force
$\vec{g}$	Acceleration due to gravity and
$G_{k,l}$	Rate of production of turbulent kinetic energy
$H$	Tank height
$k_{La}$	Mass transfer coefficient
$k$	Turbulent kinetic energy
$N$	Impeller speed
$N_{CD}$	Impeller speed of completely dispersed
$N_F$	Impeller speed of flooded
$N_R$	Impeller speed of recirculation
$N_p$	Power number
$N_{pg}$	Gas power number
$n_i$	Number of particles
$\Pi_{\varepsilon,l}$	Influence of the dispersed phase on continuous phase
$P$	Power consumption
$P_g$	Gassed power
$P_o$	Ungassed power
$\rho_l$	Liquid density
$Q_g$	Aeration rate
$Re$	Reynolds number
$R_b$	Blade area ratio

$T$	Tank internal diameter
$\bar{\bar{\tau}}_l$	Liquid phase stress-strain tensor
$\Gamma$	Torque
$U_g$	Superficial gas velocity
$\mu$	Viscosity
$\vec{u}_l$	Liquid velocity
$V$	Volume
$V_\infty$	Bubble rise velocity
$v_{sg}$	Superficial gas velocity
$\sigma$	Interfacial tension

## LIST OF ABBREVIATIONS

2D	Two dimensions
3D	Three dimensions
BDM	Bubble density model
CARPT	Computer-automated radioactive particle tracking
CFD	Computational Fluid Dynamics
CT	Computed tomography
DRW	Discrete random walk
EBI	Eddy-bubble interaction
GRT	Gamma Ray Tomography
IO	Inner-outer method
LDA	Laser Doppler Anemometry
LPM	Liter per minute
MRF	Multiple reference frame
PBM	Population balance modelling
PIV	Particle Image Velocity
RANS	Reynold averaged Navier-Stokes
RDT	Rushton turbine
rpm	Rotational per minute
SG	Sliding grid method
SN	Schiller-Naumann drag model

SR	Solidity ratio
STR	Stirred tank
UDF	User defined function

## CHAPTER 1

### INTRODUCTION

#### 1.1 Motivation

In the process industry, many unit operations are performed in stirred tanks and reactors. There are various fields like building construction; chemical manufacturing and food processing in which mixing tanks manifest themselves and commonly involving the reaction between liquid and gas phases. But, for the successful working in the industry, efficient and proper machinery or equipment are required. The good performance of stirred reactor can be achieved by making adjustment on the inappropriate operating hardware and parameters. The parameters like impeller shapes (Murthy et al., 2008; Sun et al., 2006), impeller speed (Ford et al., 2008; Taghavi et al., 2010; Wang et al., 2006; Qingbai et al., 2010; Ahmed et al., 2010), impeller position (Bakker and Akker, 1994), sparger position (Bakker and Akker, 1994), aeration rate (Bakker and Akker, 1994; Wang et al., 2006), have been studied by them experimentally and numerically. In order to design the highly performance of stirred tank, it is required for engineer to know local gas hold-up which depends on the gas and liquid properties, superficial gas velocity, sparger and impeller design and power consumption and how it changes with different operating conditions (Ford et al., 2008). Flooded is undesirable as it can lower the mass transfer in gas-liquid STR (Bakker & Akker, 1994; Xiao & Takahashi, 2007). While in the loaded regime has poor gas distribution throughout the vessel and completely dispersed regime is highly desirable operating regime due to the gas being completely dispersed at a low power input (Ford et al., 2008).

With the advancement of technology, the flow patterns inside the gas-liquid flow can readily be gained by Computational Fluid Dynamics (CFD) whereby it is not required high in cost and longer time to design the prototype or pilot scale testing compared to experiment set-up. The flow patterns of gas-liquid in STR are complicated to predict and have been studied by many authors by using the CFD (Khopkar and Ranade, 2005; Murthy et al., 2008; Gentric et al., 2005; Deen et al., 2002; Ahmed et al., 2010; Taghavi et al., 2010). Ford et al. (2008) and Heindel et al. (2008) have been used X-ray Computed Tomography to measure the local time-averaged gas hold-up in STR but this equipments is very expensive and cannot measure the different size of gas bubbles that coexist in gas-liquid STR. Nevertheless, other authors also utilized the sophisticated equipments in their experiments to measure the flow pattern in gas-liquid STR like Gamma Ray Tomography, GRT (Veera, 2001; Bukur et al., 1996), Particle Image Velocity, PIV (Deen et al., 2002; Laakonen et al., 2005), Laser Doppler Anemometry, LDA (Rutherford et al., 1996).

## 1.2 Problem Statement

In process industry, mixing tank is widely used to conduct any process that can contribute an annual turnover value of around €1370 billion worldwide, thus indicate that the importance of stirred tank reactors themselves (Butcher and Eagles, 2002). Poor mixing of stirred tank can be identified by presence of impeller flooding which has low in mass transfer coefficient ( $k_L a$ ). Extensive Experimental methods available to evaluate performance of gas-liquid STR for example Gamma Ray Tomography (GRT), Laser Doppler Anemometry (LDA) and Particle Image Velocity (PIV). However, experiment often expensive to setup due to costly instrument (i.e. PIV, GRT, LDA) and often needs long time to develop a prototype for testing (Gimbun et al., 2009). Alternatively, CFD can be employed to evaluate performance of gas-liquid STR at lower cost and in shorter time. Thus, this work attempts to evaluate gas-liquid STR performance via CFD focusing mainly on the flooding to dispersed regime transition. Therefore, the CFD model developed in this work may be useful to eliminate the impeller flooding.



### **1.3 Research Objective**

The aim of this study is to perform the Computational Fluid Dynamics (CFD) on gas-liquid stirred tank operating under flooding, loaded and fully dispersed regime with the hope the model can be applied in the future to eliminate impeller flooding that can cause poor and inefficient mixing in gas-liquid stirred tank.

### **1.4 Scope of Research**

In order to achieve the objective, this present work was study on gassed power number in gas-liquid stirred tank via CFD at various flow regimes. Besides that, gas hold-up was studied by comparing the prediction studied by Ford et al. (2008) by employed the turbulence model, Eulerian-Eulerian model and drag model for bubble in CFD at various flow regime.

### **1.5 Significance of Research**

By employing CFD simulation in this present work, it can reduce the cost of development and design the gas-liquid stirred tank instead of using the experimental method that required high cost of instruments. Besides that, this simulation can reduce the time taken to evaluate the performance of gas-liquid stirred tank in comparison with the experimental method because it can be a time-consuming in order to design the prototype and pilot scale testing of stirred tank reactors.

### **1.6 Structure of Thesis**

The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provides a description of the applications and general description on the flow characteristics of the system, as well as the dimensionless groups and correlations to account for the flow phenomena are presented. This chapter also provides a summary of

the previous study on multiphase flow or single flow via numerical simulation or experimental work. The empirical equations to be used are also presented in this chapter.

Chapter 3 gives a review of the CFD approach applied for stirred tanks modelling gas-liquid flows including the multiphase modelling, drag force modelling, turbulence modelling and impeller modelling. The modelling strategy and the tank dimension were explained briefly in this chapter. The step to conduct this CFD simulation also presented.

Chapter 4 discussed the power consumption and the gas hold-up in gas-liquid stirred tank. The time averaged of the flow was measured at different impeller speed. The result of aeration power, local gas hold-up along  $x$ -axis and average  $z$  slice hold-up were compared with predicted result and experimental data from Ford et al. (2008). This chapter also show the flow contour inside the gas-liquid stirred tank.

Chapter 5 draws together a summary of the thesis and outlines the future work which might be derived from the model developed in this work.

## **CHAPTER 2**

### **LITERATURE REVIEW**

#### **2.1 Overview**

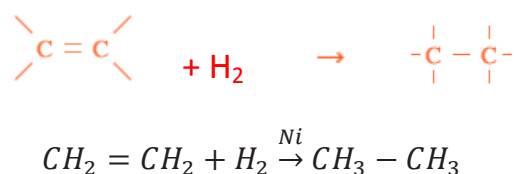
This chapter will give a brief description on the application of stirred tank in industry. Besides that, the advantages of CFD will be described and further description of three different flow regimes in gas-liquid stirred tank will be discussed. Other than that, the CFD simulation in gas-liquid stirred tank will be further discussed. Moreover, the empirical equations that will be used throughout this study will be described briefly. On the other hand, several published research on the experimental and numerical simulation method of STR will be reviewed clearly.

#### **2.2 Application of Stirred Tank**

Many chemical productions used stirred tank in process industry. They are required for carrying out any process efficiently and conveniently. It is validated with the studied made by Butcher and Eagles (2002), saying that about 50% chemical process taking place in stirred tanks and give \$1290 billion per year of profit income. This indicates that the importance of gas-liquid stirred tank in variety of chemical process such as hydrogenation, oxidation, chlorination and aerobic fermentation. Therefore, some examples of such process will be described below.

### 2.2.1 Hydrogenation

Hydrogenation process is widely applied in industry for instance pharmaceutical, petrochemical and food processing. The normal process conditions of this process involve elevated pressure and temperature in the presence of a precious metal catalyst (i.e nickel for margarine production). One example of food processing that used hydrogenation process is producing margarine or butter from a certain fatty oils; vegetables or animals. In this production, hydrogen is sparged into the bottom of the tank and will react with the carbon-carbon double bond inside the tank. The reaction is simplified as below:



**Figure 2.1:** Hydrogenation reaction

### 2.2.2 Aerobic Fermentation

For aerobic fermentation, oxygen transfer is a key variable and is a function of aeration and agitation (Potumarthi et al., 2007). This kind of process is commonly used in food and pharmaceuticals industries. Some examples of the product consist of protease enzyme (Kumar and Hiroshi, 1999), bacteria (Boodhoo et al., 2010), yeast and vitamin. The main feature of aerobic fermentation is the provision for adequate aeration; in some cases, the amount of air needed per hour is about 60-times the medium volume. Therefore, stirred tank used for aerobic fermentation have a provision for adequate supply of sterile air, which is generally sparged into the medium.

### 2.2.3 Wastewater Treatment

In wastewater treatment process, mixing tank is used to keep and mix the sludge. This is due to maintaining the sludge conditions from being septic. Therefore, sludge should be keep mixing, aerobic conditions (adequate air) must have maintained and chemicals need to be applied into the mixing tank in order to eliminate septicity and reduce odour potential in mixing tanks. The amount of air needed to mix the full tank volume is depends on the sludge.

### 2.2.4 Oxidation

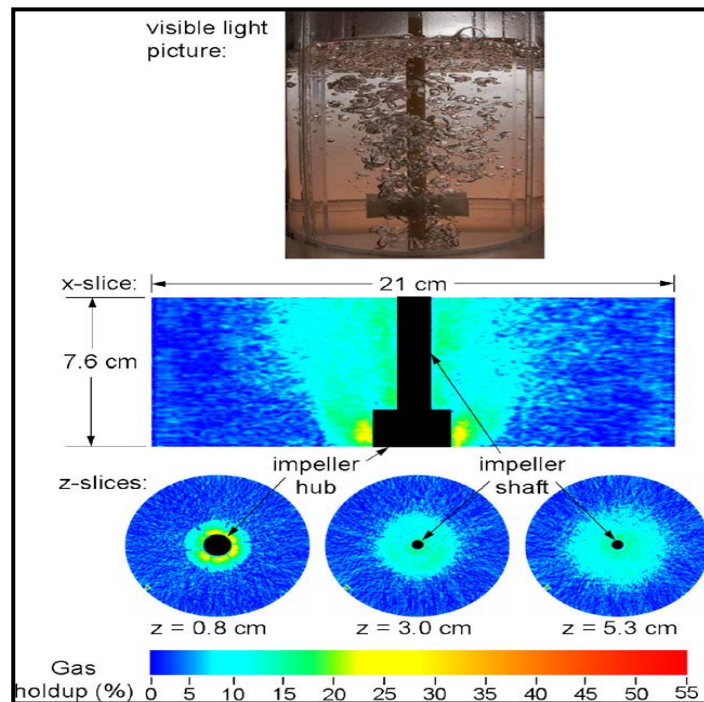
Oxidation process is widely in biological process that involved the microorganism. One example of such process carried out in aerated stirred tanks has been reported by Gomez and Cantero (2002). They reported that *Thiobacillus ferrooxidans* is an acidophilic bacterium that has the ability to oxidise ferrous to ferric iron in the presence of atmospheric oxygen and carbon dioxide and it is a dominant organism in the process of value metal extraction by microbial leaching of pyritic ores. Hence, the main purpose for the air sparging into stirred tank is to stimulate growth of bacteria (oxygen is required for respiration) for bioleaching process.

## 2.3 Flow Regime in Gas-Liquid Stirred Tank

Gas-liquid stirred tank is widely used in process industry to carry out reaction between gases and liquids. The flow patterns inside stirred tank are complicated and can be classified into four which are flooded, loaded, fully dispersed and gas recirculation. This part has been studied by many authors (Myers et al., 1994; Bombac and Zun, 2006; Ranade et al., 2008; Ford et al., 2008). Further description on the four class of flow regime will be described below. The pictures of different bulk flow pattern taken by Ford et al. (2008) can be seen at **Figure 2.2, Figure 2.4, Figure 2.5.**

### 2.3.1 Flooded Regime

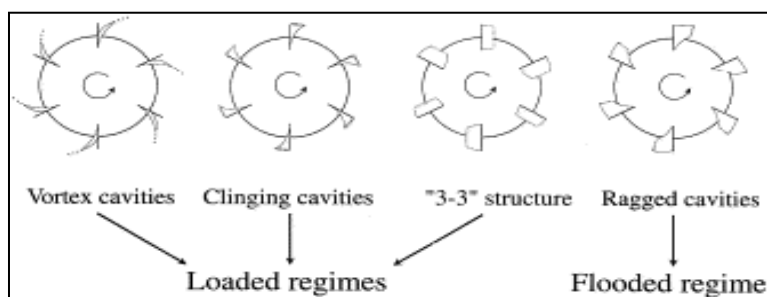
Flooded is highly undesirable in any process involve in gas-liquid stirred tank. In the presence of flooding in gas-liquid stirred tank can effect the performance of mixing because of the cavity formation behind the impeller blades. Therefore, this present work was carried out in CFD model in order to eliminate the impeller flooding. Flooding occurs when the impeller speed is low ( $0 < N < N_f$ ) and gas flow rates are high which gas flow number and gassed power number are high. These leads to low gas hold-up and low mass transfer rates (Ford et al., 2008). According to Khopkar et al. (2005), as the vertical distance increase from impeller region, the gas hold-up will be increase due to the decreasing of pressure acting on the bubble and also decreasing of bubble rise velocity. Ford et al. (2008) have been captured the flow pattern as flooded by using X-ray Computed Tomography as shown in **Figure 2.2**. They reported that  $x$ -slice compares well with the accompanying visible light picture, which also shows the large bubble size for these conditions. There are very few bubbles near the tank walls, which is common of the flooded region.



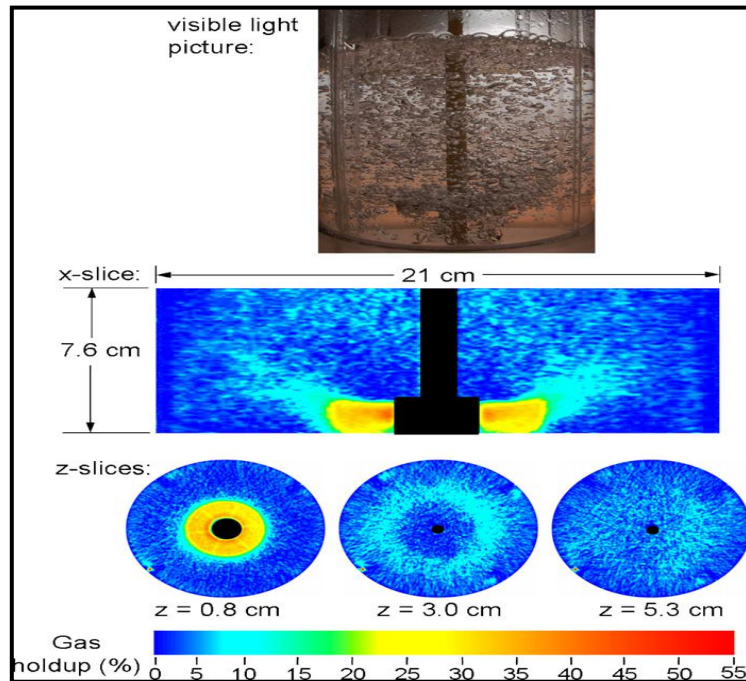
**Figure 2.2:** Flooded flow regime at  $Q_g = 9\text{LPM}$  and  $N = 200\text{ rpm}$  (Ford et al., 2008)

### 2.3.2 Loaded Regime

Loaded regime occurred as the flow transitions from flooded. Loaded pattern can be identified when the impeller speed is higher than impeller speed of flooded as well as lower than impeller speed of completely dispersed ( $N_f < N < N_{cd}$ ). The flow regime in stirred-tank reactors is strictly linked to the gas cavity structure developed behind the blades (**Figure 2.3**). The differences occurring in the cavity structure have been excellently described by Nienow et al. (1985). According to Ford et al. (2008), loaded regime is still poor gas distribution due to the buoyant forces of the gas being larger than the radial drag force resulting from the liquids mixing even the impeller at this regime is better able to radially distribute the gas. Besides that, across the transitions of flooded to loaded, the bubbles have decreased in size and are located throughout a larger region of the stirred tank as shown by visible light picture (**Figure 2.4**). In fact there are very few bubbles below the impeller as well as defined as the characteristics of loaded.



**Figure 2.3:** Cavity structure at loaded and flooded regime

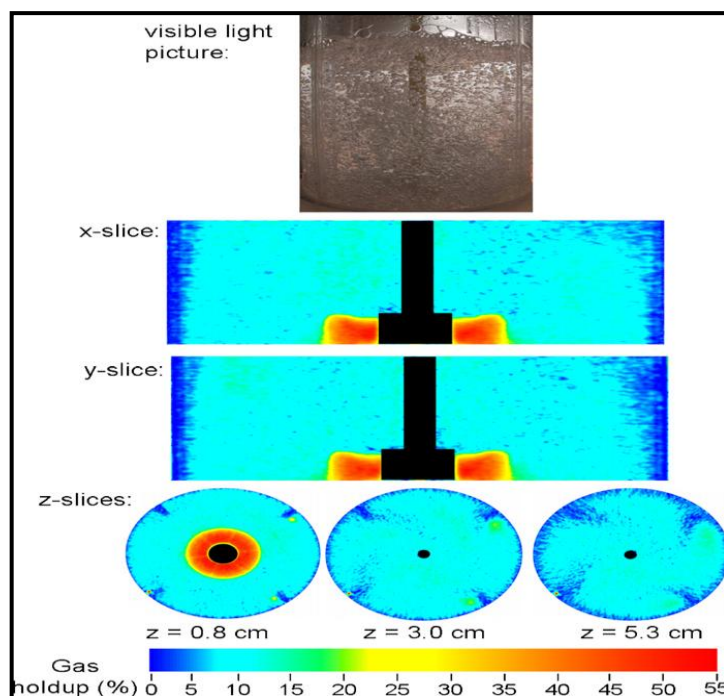


**Figure 2.4:** Loaded flow regime at  $Q_g = 9\text{LPM}$  and  $N = 350\text{ rpm}$  (Ford et al., 2008)

### 2.3.3 Fully Dispersed Regime

Fully dispersed regime or completely dispersed regime is highly desirable operating regime due to the gas being completely dispersed in at lower power input. If ( $N_{cd} < N < N_r$ ), the flow is falls into the fully dispersed regime due to the increased of impeller's angular velocity. As reported by Ford et al. (2008), the CT images show high gas holdups throughout the entire imaging region, which are higher than those for the other two conditions; flooded and loaded. As shown by the visible light picture (**Figure 2.5**), bubbles have further decreased in size and they are located throughout the stirred tank. If the impeller speed is increased still further, gas recirculation can be observed ( $N = N_r$ ) (Paglianti et al., 2000).





**Figure 2.5:** Completely dispersed flow regime at  $Q_g = 9\text{LPM}$ ,  $N = 700$  rpm

(Ford et al., 2008)

## 2.4 CFD Simulation

The CFD simulation is used to portray hydrodynamics behaviour in the reactor, including the velocity field, biogas volume fraction, turbulence kinetic energy and shear strain rate. Due to the progress in computer technology CFD seems now able to deal with industrial applications at moderate costs and turnaround times. The future relevance of CFD will therefore depend on how accurate complex flows can be calculated. Since many flows of engineering interest are turbulent, the appropriate treatment of turbulence will be crucial to the success of CFD (Sodja, 2007). Configuration optimization of the reactor is achieved by optimizing the impeller design. In the last two decades, computational fluid dynamics (CFD) has become known as a potential tool for ‘a priori prediction’ of the flow field in the stirred reactors. The CFD based models were shown to be successful in